

10/787, 375

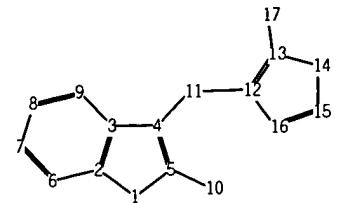
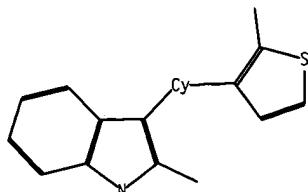
(FILE 'HOME' ENTERED AT 16:35:24 ON 30 NOV 2004)

FILE 'REGISTRY' ENTERED AT 16:35:37 ON 30 NOV 2004

L1 STRUCTURE UPLOADED
L2 QUE L1
L3 STRUCTURE UPLOADED
L4 QUE L3
L5 3 S L2
L6 95 S L2 FULL
L7 3 S L4
L8 95 S L4 FULL
L9 95 S L6 OR L8

FILE 'CAPLUS' ENTERED AT 16:36:38 ON 30 NOV 2004

L10 71 S L9 FULL
L11 71 S L10 AND PY <= 2004
L12 1 S L11 AND SIDE-CHAIN
L13 0 S L11 AND PENDAN?
L14 0 S L11 AND PENDANT
L15 6 S L11 AND CHAIN
L16 0 S L11 AND BACKBONE



chain nodes :

10 11 17

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16

chain bonds :

4-11 5-10 11-12 13-17

ring bonds :

1-2 1-5 2-3 2-6 3-4 3-9 4-5 6-7 7-8 8-9 12-13 12-16 13-14
14-15 15-16

exact/norm bonds :

1-2 1-5 3-4 4-5 4-11 11-12 12-13 12-16 13-14 14-15 15-16

exact bonds :

5-10 13-17

normalized bonds :

2-3 2-6 3-9 6-7 7-8 8-9

Match level :

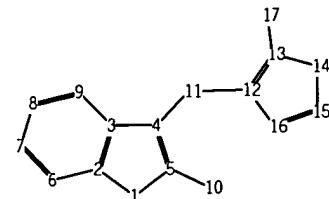
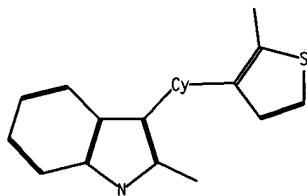
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS

Generic attributes :

11:

Saturation : Unsaturated

Type of Ring System : Monocyclic



chain nodes :

10 11 17

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16

chain bonds :

4-11 5-10 11-12 13-17

ring bonds :

1-2 1-5 2-3 2-6 3-4 3-9 4-5 6-7 7-8 8-9 12-13 12-16 13-14
14-15 15-16

exact/norm bonds :

1-2 1-5 3-4 4-5 4-11 11-12 12-13 12-16 13-14 14-15 15-16

exact bonds :

5-10 13-17

normalized bonds :

2-3 2-6 3-9 6-7 7-8 8-9

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS

Generic attributes :

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Saturation : Unsaturated

Type of Ring System : Monocyclic